

Quantum open systems approach to current noise in resonant tunnelling junctions.

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Abstract

A quantum Markovian master equation is derived to describe the current noise in resonant tunnelling devices. This equation includes both incoherent and coherent quantum tunnelling processes. We show how to obtain the population master equation by adiabatic elimination of quantum coherences in the presence of elastic scattering. We calculate the noise spectrum for a double well device and predict sub-shot noise statistics for strong tunnelling between the wells. The method is an alternative to Green's functions methods, and population master equations for very small coherently coupled quantum dots.

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I. INTRODUCTION

Quantum features of conductance in mesoscopic electronics is currently a major theoretical and experimental research interest in condensed matter physics [1]. Developments are driven by two complementary imperatives. Firstly a technological trend to fabricate devices on smaller and smaller scales is rapidly approaching the point where quantum effects will become a problem unless explicit attempts to exploit quantum features are made. Quantum tunnelling can lead to undesired coupling between fabricated structures. On the other hand, tunnelling offers the possibility of very fast switching times. Secondly, the new devices require improvements to the theoretical description of electronic transport in a low temperature, high mobility regime. Small devices with very long coherence times can be dominated by coherent quantum effects. It is becoming increasingly clear that intrinsic quantum fluctuations play an important role at low temperatures [2]

Current noise in resonant tunnelling devices (RTD) provides a path to understanding noise in the deep quantum domain. In a biased RTD one or more bound quantum states are coupled incoherently to two electron reservoirs maintained at different chemical potential. There are a number of experimental [3–6] and theoretical [7–12] results. RTDs involve exchange of fermions between the reservoirs, and the bound states. We propose in this paper an approach to such devices based on quantum markov master equations [13]. Such an approach to quantum noise in nonequilibrium systems has been used with great success in quantum optics. This provides an alternative approach to the conventional Green’s functions methods, and offers additional physical insights. For example it enables one to deal with coherent coupling between adjacent well states which couples off-diagonal elements of the density matrix in the occupation number basis and cannot be described by population master equations. Such coupling can occur in strongly coupled quantum dots, as in the recent experiments of Blick et al [14] and Oosterkamp et al [15].

If the strength of this coherent coupling dominates the time scales of elastic and inelastic relaxation, a population master equation cannot describe the system. Coherently coupled

Nanostructures are likely to become increasingly important and thus there is considerable motivation to develop theoretical schemes that go beyond population rate equations.

In the first part of this paper we derive the operator master equation to describe a bound electronic system coupled incoherently to two reservoirs. We then apply this equation to calculate the current two-time correlation function for a single well, with a single bound state. This model of course can equally well be treated by a population master equation approach as in the approach of Carlos Egues et al. [16], but we rederive the known results simply to display the method in a familiar context. In section III we apply our methods to treat the case of coherent coupling between the bound states of adjacent wells. In this case our approach yields results that go beyond the traditional population master equation approach. We derive the current spectrum in the device and demonstrate new features that arise precisely because of the coherent coupling between the two wells. To make contact with previous work we show that in the limit when elastic scattering dominates the coherent coupling, a population rate equation may be derived that is equivalent, in the appropriate limit, to that obtained by Carlos Egues et al. [16].

II. THE MASTER EQUATION

We begin with the derivation of the master equation for a single quantum tunnelling channel connecting two reservoirs under external bias. This system is quite adequately described by other methods, including population master equations. However we treat it here simply to demonstrate our approach in a familiar setting. Therefore our results are not new and could equally well be obtained by other methods. This is not the case for the coherently coupled double well system we discuss next. The hamiltonian describing this process is given by [9]

$$\begin{aligned}
 H = & \sum_k \varepsilon_k^E a_k^\dagger a_k + \varepsilon_c c^\dagger c + \sum_p \varepsilon_p^C b_p^\dagger b_p \\
 & + \sum_k (T_{Ek} c^\dagger a_k + T_{Ek}^* a_k^\dagger c)
 \end{aligned}
 \tag{1}$$

$$+ \sum_p (T_{Cp} b_p^\dagger c + T_{Cp}^* c^\dagger b_p)$$

where $a_k(a_k^\dagger)$, $c(c^\dagger)$ and $b_p(b_p^\dagger)$ are the annihilation (creation) operators of electrons in the emitter (E) reservoir, in the central quantum well and in the collector (C) reservoir respectively. The energy of the bound state without bias is ε_0 which under bias becomes $\varepsilon_c = \varepsilon_0 - \alpha eV$ where α is a structure dependent coefficient. The single particle energies in the emitter and collector are respectively, $\varepsilon_k^E = k^2/2m$ and $\varepsilon_p^C = p^2/2m - eV$. The energy reference is at the bottom of the conduction band of the emitter reservoir.

The fourth and fifth terms in the Hamiltonian describe the coupling between the quasibound electrons in the well and the electrons in the reservoir. The tunnelling coefficients T_{Ek}, T_{Cp} depend on the barrier profile and the bias voltage. We will assume that at all times the two reservoirs remain in thermal equilibrium, with chemical potentials μ_C, μ_E , with $\mu_E - \mu_C = eV$, despite the tunnelling of electrons. This is one of the key defining characteristics of a reservoir. It assumes in effect that two very different time scales describe the dynamics of the reservoirs and the quasibound quantum state in the well.

In the interaction picture the Hamiltonian may be written as

$$H_I(t) = \hbar \sum_{i=1}^2 (c^\dagger \Gamma_i(t) e^{i\omega_0 t} + c \Gamma_i^\dagger(t) e^{-i\omega_0 t}) \quad (2)$$

where the bound state frequency is $\omega_0 = \varepsilon_c/\hbar$ and the reservoir operators are given by

$$\Gamma_1(t) = \sum_k T_{Ek} a_k e^{-i\omega_k^E t} \quad (3)$$

$$\Gamma_2(t) = \sum_p T_{Cp} b_p e^{-i\omega_p^C t} \quad (4)$$

where

$$\omega_k^E = \frac{\varepsilon_k^E}{\hbar} \quad (5)$$

$$\omega_p^C = \frac{\varepsilon_p^C}{\hbar} \quad (6)$$

We now obtain an equation of motion for the density operator of the bound state, $\rho(t)$, in the well following the standard method based on second order perturbation theory and tracing over reservoir states [17]. Thus we need

$$\frac{d\rho(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt_1 Tr_R[H_I(t), [H_I(t_1), \rho_R \otimes \rho(t)]] \quad (7)$$

where ρ_R is the thermal equilibrium state of the two reservoirs, and Tr_R denotes a trace over the reservoir variables. Note that the factorisation of the well state and reservoir states has been assumed. This is reasonable if the well state and the reservoir states are initially uncorrelated and provided there is a wide separation in the relaxation time scales of the well state and the reservoirs. The only non zero correlation functions we need to compute are

$$I_{E1}(t) = \int_0^t dt_1 \langle \Gamma_1^\dagger(t_1) \Gamma_1(t_1) \rangle e^{-i\omega_0(t-t_1)} \quad (8)$$

$$I_{E2}(t) = \int_0^t dt_1 \langle \Gamma_1(t_1) \Gamma_1^\dagger(t_1) \rangle e^{-i\omega_0(t-t_1)} \quad (9)$$

$$I_{C1}(t) = \int_0^t dt_1 \langle \Gamma_2^\dagger(t_1) \Gamma_2(t_1) \rangle e^{-i\omega_0(t-t_1)} \quad (10)$$

$$I_{C2}(t) = \int_0^t dt_1 \langle \Gamma_2(t_1) \Gamma_2^\dagger(t_1) \rangle e^{-i\omega_0(t-t_1)} \quad (11)$$

In order to illustrate the important physical approximations required in deriving the master equation we will now explicitly evaluate the first of these correlation functions.

Using the definition of the reservoir operators and the assumed thermal Fermi distribution of the electrons in the emitter we find

$$I_{E1}(t) = \sum_k \bar{n}_{Ek} |T_{Ek}|^2 \int_0^t dt_1 e^{i(\omega_k^E - \omega_0)t} \quad (12)$$

As the reservoir is a large system by definition we can replace the sum over k by an integral to obtain

$$I_{E1}(t) = \int_0^\infty \frac{d\omega}{2\pi} \rho(\omega) \bar{n}(\omega) |T_E(\omega)|^2 \int_0^\tau d\tau e^{i(\omega - \omega_0)\tau} \quad (13)$$

where we have changed the variable of time integration. The dominant term in the frequency integration will come from frequencies near ω_0 as the time integration is significant at that point. We assume that the bias is such that the quasibound state is well below the Fermi level in the emitter. This implies that near $\omega = \omega_0$, the average occupation of the reservoir state is very close to unity. This is an effective low temperature approximation. Now we make the first Markov approximation. We assume that the function $\rho(\omega) \bar{n}(\omega) |T_E(\omega)|^2$ is

slowly varying around $\omega = \omega_0$, and thus the frequency integration will lead to a function which is a rapidly decaying function of time compared to dynamical time scales for the quasibound state. This implies that on time scales of interest in an experiment we can extend the upper limit of the time integration to infinity as a good approximation. In that case I_{E1} becomes time independent and may be approximated by

$$\begin{aligned} I_{E1}(t) &\approx \int_0^\infty \frac{d\omega}{2} \rho(\omega) |T_E|^2 \delta(\omega_0) \\ &= \gamma_L(\omega_0) \end{aligned} \quad (14)$$

which defines the effective rate γ_L of injection of electrons from the left reservoir (the emitter) into the quasibound state of the well. This rate will have a complicated dependence on the bias voltage through both ω_0 and the coupling coefficients $|T_E(\omega)|$. In this paper we do not address this issue. We simply seek the noise properties as a function of the rate constants.

Evaluating all the other correlation functions under similar assumptions we find that the quantum master equation for the density operator representing the well-state in interaction picture is given by

$$\begin{aligned} \frac{d\rho}{dt} &= \mathcal{L}\rho \\ &= \frac{\gamma_L}{2} (2c^\dagger \rho c - cc^\dagger \rho - \rho cc^\dagger) \\ &\quad + \frac{\gamma_R}{2} (2c \rho c^\dagger - c^\dagger c \rho - \rho c^\dagger c), \end{aligned} \quad (15)$$

γ_L and γ_R are constants determining the rate of injection of electrons from emitter into the well and from the well into the collector respectively. The rate constants can be determined by a self-consistent band calculation involving the bias voltage. Two Poisson processes shown in the master equations: the injection of electrons into the well described by the first term in the right hand and the emission of electrons out of the well by the second term, are conditioned by the rates $\gamma_L \langle cc^\dagger \rangle(t)$ and $\gamma_R \langle c^\dagger c \rangle(t)$:

$$E(dN_E(t)) = \gamma_L \langle cc^\dagger \rangle dt; E(dN_C(t)) = \gamma_R \langle c^\dagger c \rangle dt \quad (16)$$

where the average is taken with respect to the well state at any time t . The master equation

15 is diagonal in the occupation number representation. The mean occupation number $\bar{n} = \text{Tr}(c^\dagger c \rho(t))$ can therefore be determined easily from the rate equation

$$\frac{d\bar{n}}{dt} = \gamma_L(1 - \bar{n}) - \gamma_R\bar{n} \quad (17)$$

However the occupation number of the well states is not directly measured in current experiments. The current noise is a fluctuation in classical stochastic processes. It is measured in the relatively high temperature reservoirs of the leads, well away from the well state, and the strong, fast electron-electron interactions in the reservoir establish the classical level of the observed variable. It is however conditioned on the underlying quantum stochastic process in the well, which is described by the master equation. We thus have the familiar problem of connecting the observed classical stochastic process to the quantum source of information in an open quantum system. In this problem we proceed as follows. The current pulse in the emitter and collector may be determined from the Ramo-Shockley theorem [18]. For a symmetric geometry this takes the form,

$$i(t)dt = \frac{e}{2} (dN_E(t) + dN_C(t)) \quad (18)$$

The connection to the quantum source is then made by equations (16). Using Eq(16), the average current is given by $E(i(t)) = \gamma_L(1 - \bar{n}) - \gamma_R\bar{n}$. In the steady state this is $i_\infty = \frac{e\gamma_L\gamma_R}{\gamma}$ where $\gamma = \gamma_L + \gamma_R$ and the subscript ∞ indicates the steady state.

The fluctuations in the observed current, $i(t)$ are quantified by the two-time correlation function:

$$G(\tau) = \frac{e}{2} i_\infty \delta(\tau) + \langle I(t), I(t + \tau) \rangle_\infty^{\tau \neq 0} \quad (19)$$

To relate these classical averages to the fundamental quantum processes occurring in the well we apply the theory of open quantum system [19] to the present system and calculate the following correlation components with $\tau > 0$ [20]:

$$E(dN_E(t + \tau)dN_E(t)) = \gamma_L^2 \text{Tr}(cc^\dagger e^{\mathcal{L}\tau} c^\dagger \rho_\infty c) dt^2 \quad (20)$$

$$E(dN_C(t+\tau)dN_C(t)) = \gamma_R^2 Tr(c^\dagger c e^{\mathcal{L}\tau} c \rho_\infty c^\dagger) dt^2 \quad (21)$$

$$E(dN_E(t+\tau)dN_C(t)) = \gamma_L \gamma_R Tr(cc^\dagger e^{\mathcal{L}\tau} c \rho_\infty c^\dagger) dt^2 \quad (22)$$

$$E(dN_C(t+\tau)dN_E(t)) = \gamma_R \gamma_L Tr(c^\dagger c e^{\mathcal{L}\tau} c^\dagger \rho_\infty c) dt^2 \quad (23)$$

Calculating the above correlation components using master equation with corresponding initial conditions, and substituting them together with the shot-noise component into equation 19 yield:

$$G(\tau) = \frac{ei_\infty}{2}\delta(\tau) + \frac{ei_\infty}{4}\left(1 - \frac{4\gamma_L\gamma_R}{\gamma^2}\right)\gamma e^{-\gamma|\tau|} \quad (24)$$

Thus the spectral density of current fluctuation in frequency domain is given by

$$\begin{aligned} S(\omega) &= 2 \int_0^\infty G(\tau) (e^{i\omega\tau} + e^{-i\omega\tau}) d\tau \\ &= ei_\infty \left(1 + \left(1 - \frac{4\gamma_L\gamma_R}{\gamma^2}\right) \frac{\gamma^2}{\gamma^2 + \omega^2}\right) \end{aligned} \quad (25)$$

The current Fano factor $F(\omega)$ is defined as the ratio of current noise density over the full shot noise density, and for low frequencies ($\gamma \gg \omega$):

$$F(0) = \frac{S(0)}{2ei_\infty} = 1 - \frac{2\gamma_L\gamma_R}{\gamma^2} \quad (26)$$

The shot noise is suppressed and reaches the minimum of 50 % in a symmetric structure with $\gamma_L = \gamma_R$. The result is same as those derived by Chen and Ting [9] using non-equilibrium Green's function method. The result can also be obtained by a classical master equation calculation [10]. However the classical master equation cannot be used to treat the case of coherent coupling in a double well system discussed below.

The suppression of fluctuations at low frequency is due to the exclusion principle in the well state, reflected in the master equation by the appearance of the anti-commuting field operators. No electron can tunnel onto the well if an electron is already there. We need to wait a time of the order of γ^{-1} for the electron to tunnel back out into the collector. Thus

strong anti-correlations are established in the two fundamental Poisson processes, $dN_i(t)$. If the tunnelling particles were bosons, the well could accumulate a large number of particles, enhancing the probability for emission into the collector. This would lead to a rapid bunching of emission events into the collector and a super-shot noise current would result. At high frequencies, we are looking at fast processes in which an electron tunnels into the well and immediately tunnels out. The Fano factor at high frequencies is 0.5 due to the assumed form of Ramo-Shockley theorem.

III. NOISE PROPERTIES OF A COHERENTLY COUPLED DOUBLE WELL STRUCTURE

We now apply our approach to a triple barrier and double quantum well involving elastic scattering within the wells and coherent coupling between the wells. The main procedures are parallel to those in single well case but now involve off-diagonal elements of the density matrix. The master equation is,

$$\begin{aligned}
\frac{d\rho}{dt} = & \frac{\gamma_L}{2} \left(2c_1^\dagger \rho c_1 - c_1 c_1^\dagger \rho - \rho c_1 c_1^\dagger \right) \\
& + \frac{\gamma_R}{2} \left(2c_2^\dagger \rho c_2 - c_2 c_2^\dagger \rho - \rho c_2 c_2^\dagger \right) \\
& - \eta_1 \left[c_1^\dagger c_1, \left[c_1^\dagger c_1, \rho \right] \right] \\
& - \eta_2 \left[c_2^\dagger c_2, \left[c_2^\dagger c_2, \rho \right] \right] \\
& - i\Omega \left[(c_1^\dagger c_2 + c_2^\dagger c_1), \rho \right]
\end{aligned} \tag{27}$$

where $c_1(c_1^\dagger)$ and $c_2(c_2^\dagger)$ are annihilation (creation) operator of electron in the left and right quantum well respectively, η_i is the rate of elastic scattering (electron-phonon for example) in the i th well, and Ω is the coherent coupling rate between the two well states. The irreversible term describing the elastic scattering is derived in much the same way as the inelastic tunnelling terms that describe electrons entering and leaving the device, with one additional assumption. To get a Markov master equation for number conserving scattering events we must assume that the temperature of the bath describing such processes is high

enough that the bath states are well away from the ground states. This is not a very restrictive assumption for realistic devices at milliKelvin temperatures. The deviations that can result for very low temperatures are described in Gardiner [13] The derivation of the scattering term in the master equation (27) is detailed in the appendix.

The last term in this equation represents a coherent coupling between the two wells and causes a single electron to periodically tunnel backward and forward between the two wells, until it is eventually lost through the final barrier. Recently Blick et al [14], have made measurements on a structure that can be roughly approximated by our model. As they point out this device exhibits a new feature, in that a single electron can be in a superposition state between the two wells and is thus like an artificial molecule. We first derive the noise features in the presence of this coherent coupling. We will then show that, in the limit of strong elastic scattering, $\eta_i \gg \Omega$, the system can be described in terms of population rate equations that have been extensively used in the past.

The steady state current is easily found to be given by

$$i_\infty = \frac{2e\Omega^2\gamma_e}{\gamma_e^2 + 2\gamma_e\eta_e + 4\Omega^2} \quad (28)$$

for a symmetric system, $\gamma_L = \gamma_R \equiv \gamma_e$; $\eta_1 = \eta_2 \equiv \eta_e$. The appropriate correlation functions may be evaluated to give,

$$\begin{aligned} \langle I(t), I(t+\tau) \rangle_\infty &= \left(\frac{e\gamma_e\Omega}{\lambda_+\lambda_-} \right)^2 \left\{ 4\Omega^2 \right. \\ &\quad \left. + \frac{1}{4\Delta} [f_+e^{\lambda_+\tau} + f_-e^{\lambda_-\tau}] \right\} \end{aligned} \quad (29)$$

where

$$f_\pm = (\gamma_e - \eta_e \pm \Delta) (\Delta \pm \eta_e) (\gamma_e + \eta_e + \Delta) \quad (30)$$

and $\Delta \equiv \sqrt{\eta_e^2 - 4\Omega^2}$; $\lambda_\pm = -\gamma_e - \eta_e \pm \Delta$. The noise spectra are derived in two cases. In case1: $\eta_e^2 > 4\Omega^2$, when the elastic scattering rate, η_i , is higher than the coherent coupling rate between the well states, the current noise spectrum is

$$S(\omega) = 2ei_\infty \left\{ \frac{1}{2} + \frac{\gamma_e}{4\Delta} \left[\frac{(\eta_e + \Delta)(\gamma_e - \eta_e + \Delta)}{(-\gamma_e - \eta_e + \Delta)^2 + \omega^2} + \frac{(-\eta_e + \Delta)(\gamma_e - \eta_e - \Delta)}{(-\gamma_e - \eta_e - \Delta)^2 + \omega^2} \right] \right\} \quad (31)$$

The current Fano factor against normalised frequency is plotted in Fig. 1 where the spectrum shows Lorentzian feature. In case2: $\eta_e^2 < 4\Omega^2$, the opposite situation, when coherent coupling is much stronger than elastic scattering, the noise spectrum

$$S(\omega) = 2ei_\infty \left\{ \frac{1}{2} + \frac{\gamma_e}{\tilde{\Delta}} \Im \left[\frac{(\gamma_e - \eta_e + i\tilde{\Delta})(\eta_e + i\tilde{\Delta})}{(-\gamma_e - \eta_e + i\tilde{\Delta})^2 + \omega^2} \right] \right\} \quad (32)$$

where $\tilde{\Delta} = \sqrt{4\Omega^2 - \eta_e^2}$, is symmetrically double peaked about the free particle frequency ($\omega = 0$) as shown in the Fig. 2. A comparison of these two quantum processes is shown in Fig. 3. When elastic scattering increases, the Fano factor increases. Increasing the coherent coupling results in noise suppression and the double peak feature are more significant as the two well coupling and the quantum correlations are stronger. Further when elastic scattering is extremely weak: $\eta_e \rightarrow 0$, and coherent coupling is strong: $\Omega \gg \gamma_e$, the steady state current $i_\infty \rightarrow \frac{e\gamma_e}{2}$ approaches the single well case as expected in this limit. A significant outcome is that the best noise reduction at low frequency when $\eta_e = 0$ reaches 0.22.

The coherent tunnelling between the two wells has a strong effect on the noise characteristics. Electrons are periodically transferred between the two wells at the tunnelling frequency. If an electron from the emitter is injected into the first well, no further electrons can enter this well until this electron is removed, which takes place on a time scale determined by Ω^{-1} . Thus at frequencies smaller than Ω , noise is suppressed by the exclusion principle, just as for the single well case. At the tunnel frequency however we expect the noise to increase, as electrons injected into the first well are quickly cycled to the second well, where they can incoherently escape to the collector. This explains the two peaked structure of the noise power spectrum. In the case of large Ω however, coherent coupling dominates. In that case if an electron tunnels into the first well it periodically returns to that well at a frequency of 2Ω . To see this it is sufficient to note that the two levels which are degenerate in the absence of tunnelling become split into symmetric and anti symmetric

combinations, separated in energy by $2\hbar\Omega$. A state initially localised in one well can then be written as a linear combination of the two new eigenstates. The phase difference in the superposition rotates through π at the frequency Ω which leads to a state localised in the other well. This is just the standard description of tunnelling in a two state system. The periodic of return of the electron to the first well suppresses another electron from entering the well. Thus at large values of Ω we expect noise suppression to occur at $\omega = 2\Omega$. This behaviour is indeed seen in figure 4.

We now show that in the limit of strong elastic scattering $\eta_i \gg \Omega$ (Case 1 above), a population master equation can be derived that describes a classical sequential tunnelling structure. The sequential model is traditionally formulated in terms of a classical master equation for the occupation probabilities of each well. In our case, we have restricted the discussion to a single bound state in each well and thus the maximum population in each well is unity. However we can derive an equivalent classical master equation to describe sequential tunnelling even in this case.

Our method is an extension of adiabatic methods used in quantum optics to obtain rate equations. We assume that the off-diagonal elements of the double well density operator are rapidly damped due to the elastic scattering rates η_i . The off-diagonal elements are then assumed to relax almost instantaneously to their steady state values and adiabatically follow the more slowly changing diagonal matrix elements.

From Eq(27) we find the following equations of motion for the matrix elements in the occupation number basis for each well,

$$\begin{aligned}
& \frac{d}{dt} \langle n_1 n_2 | \rho | m_1 m_2 \rangle \\
&= \left\{ \begin{aligned} & -\frac{\gamma_L}{2} [(n_1 + 1)\delta_{n_1,0} + (m_1 + 1)\delta_{m_1,0}] - \frac{\gamma_R}{2} (n_2\delta_{n_2,1} + m_2\delta_{m_2,1}) \\ & -\eta_1 (n_1^2\delta_{n_1,1} - 2n_1m_1\delta_{n_1,1}\delta_{m_1,1} + m_1^2\delta_{m_1,1}) \\ & -\eta_2 (n_2^2\delta_{n_2,1} - 2n_2m_2\delta_{n_2,1}\delta_{m_2,1} + m_2^2\delta_{m_2,1}) \end{aligned} \right\} \langle n_1 n_2 | \rho | m_1 m_2 \rangle \\
&+ \gamma_L \delta_{n_1,1} \delta_{m_1,1} \sqrt{n_1 m_1} \langle n_1 - 1, n_2 | \rho | m_1 - 1, m_2 \rangle \\
&+ \gamma_R \delta_{n_2,0} \delta_{m_2,0} (-1)^{n_1+m_1} \sqrt{(n_2 + 1)(m_2 + 1)} \langle n_1, n_2 + 1 | \rho | m_1, m_2 + 1 \rangle
\end{aligned}$$

$$\begin{aligned}
& -i\Omega\{\delta_{n_1,1}\delta_{n_2,0}(-1)^{n_1-1}\sqrt{n_1(n_2+1)}\langle n_1-1, n_2+1|\rho|m_1m_2\rangle \\
& +\delta_{n_1,0}\delta_{n_2,1}(-1)^{n_1}\sqrt{(n_1+1)n_2}\langle n_1+1, n_2-1|\rho|m_1m_2\rangle \\
& -\delta_{m_1,0}\delta_{m_2,1}(-1)^{m_1}\sqrt{(m_1+1)m_2}\langle n_1, n_2|\rho|m_1+1, m_2-1\rangle \\
& -\delta_{m_1,1}\delta_{m_2,0}(-1)^{m_1-1}\sqrt{(m_2+1)m_1}\langle n_1, n_2|\rho|m_1-1, m_2+1\rangle\}
\end{aligned}$$

where n_1, n_2 refer to the occupation number of the first and second wells respectively.

Note that the diagonal matrix elements represent the occupation probabilities of each well,

$$P(n_1, n_2, t) = \langle n_1, n_2 | \rho(t) | n_1, n_2 \rangle \quad (33)$$

The diagonal matrix elements then obey the equation,

$$\begin{aligned}
& \frac{d}{dt} \langle n_1 n_2 | \rho | n_1 n_2 \rangle \\
& = [-\gamma_L(n_1+1)\delta_{n_1,0} - \gamma_R n_2 \delta_{n_2,1}] \langle n_1 n_2 | \rho | n_1 n_2 \rangle \\
& + \delta_{n_1,1} \gamma_L n_1 \langle n_1-1, n_2 | \rho | n_1-1, n_2 \rangle \\
& + \delta_{n_2,0} \gamma_R (n_2+1) \langle n_1, n_2+1 | \rho | n_1, n_2+1 \rangle \\
& + i(-1)^{n_1} \Omega \{ \delta_{n_1,1} \delta_{n_2,0} \sqrt{n_1(n_2+1)} [\langle n_1-1, n_2+1 | \rho | n_1 n_2 \rangle - \langle n_1, n_2 | \rho | n_1-1, n_2+1 \rangle] \\
& + \delta_{n_1,0} \delta_{n_2,1} \sqrt{(n_1+1)n_2} [\langle n_1, n_2 | \rho | n_1+1, n_2-1 \rangle - \langle n_1+1, n_2-1 | \rho | n_1 n_2 \rangle] \}
\end{aligned}$$

we now define the off-diagonal matrix elements as

$$Y_1 \equiv \langle n_1, n_2 | \rho | n_1+1, n_2-1 \rangle$$

$$Y_2 \equiv \langle n_1, n_2 | \rho | n_1-1, n_2+1 \rangle$$

$$Y_3 \equiv \langle n_1-1, n_2+1 | \rho | n_1+1, n_2-1 \rangle$$

Therefore, the population equation we are interested is,

$$\begin{aligned}
& \frac{d}{dt} P(n_1, n_2, t) \\
& = [-\gamma_L(n_1+1)\delta_{n_1,0} - \gamma_R n_2 \delta_{n_2,1}] P(n_1, n_2, t) \\
& + \delta_{n_1,1} \gamma_L n_1 P(n_1-1, n_2, t) + \delta_{n_2,0} \gamma_R (n_2+1) P(n_1, n_2+1, t) \\
& - 2\Omega(-1)^{n_1} [\delta_{n_1,0} \delta_{n_2,1} \sqrt{(n_1+1)n_2} \text{Im } Y_1 - \delta_{n_1,1} \delta_{n_2,0} \sqrt{n_1(n_2+1)} \text{Im } Y_2]
\end{aligned}$$

Note that the elastic scattering rates, η_1, η_2 , do not directly enter this equation. This is because elastic scattering does not change the occupation of the well states but does disrupt the phase coherence between the wave functions in the wells. This will lead to a decay of the relevant off-diagonal matrix elements, which obey the equations,

$$\begin{aligned}
\frac{d}{dt}Y_1(t) &= \frac{d}{dt} \langle n_1 n_2 | \rho | n_1 + 1, n_2 - 1 \rangle \\
&= \left\{ -\frac{\gamma_L}{2}(n_1 + 1)\delta_{n_1,0} - \frac{\gamma_R}{2}n_2\delta_{n_2,1} - \eta_1[n_1^2\delta_{n_1,1} + (n_1 + 1)^2\delta_{n_1+1,1}] - \eta_2n_2^2\delta_{n_2,1} \right\} Y_1(t) \\
&\quad - i(-1)^{n_1-1}\Omega\delta_{n_1,1}\delta_{n_2,0}\sqrt{n_1(n_2 + 1)}Y_3(t) \\
&\quad - i(-1)^{n_1}\Omega\delta_{n_1,0}\delta_{n_2,1}\sqrt{(n_1 + 1)n_2}P(n_1 + 1, n_2 - 1, t) \\
&\quad + i(-1)^{n_1}\Omega\delta_{n_1+1,1}\delta_{n_2-1,0}\sqrt{(n_1 + 1)n_2}P(n_1, n_2, t)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt}Y_2(t) &= \frac{d}{dt} \langle n_1 n_2 | \rho | n_1 - 1, n_2 + 1 \rangle \\
&= \left\{ -\frac{\gamma_L}{2}[(n_1 + 1)\delta_{n_1,0} + n_1\delta_{n_1-1,0}] - \frac{\gamma_R}{2}[n_2\delta_{n_2,1} + (n_2 + 1)\delta_{n_2+1,1}] \right. \\
&\quad \left. - \eta_1n_1^2\delta_{n_1,1} - \eta_2[n_2^2\delta_{n_2,1} + (n_2 + 1)^2\delta_{n_2+1,1}] \right\} Y_2(t) \\
&\quad - i(-1)^{n_1}\Omega\delta_{n_1,0}\delta_{n_2,1}\sqrt{(n_1 + 1)n_2}Y_3^*(t) \\
&\quad - i(-1)^{n_1-1}\Omega\delta_{n_1,1}\delta_{n_2,0}\sqrt{n_1(n_2 + 1)}P(n_1 - 1, n_2 + 1, t) \\
&\quad + i(-1)^{n_1-1}\Omega\delta_{n_1-1,0}\delta_{n_2+1,1}\sqrt{n_1(n_2 + 1)}P(n_1, n_2, t)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt}Y_3(t) &= \frac{d}{dt} \langle n_1 - 1, n_2 + 1 | \rho | n_1 + 1, n_2 - 1 \rangle \\
&= \left[-\frac{\gamma_L}{2}n_1\delta_{n_1-1,0} - \frac{\gamma_R}{2}(n_2 + 1)\delta_{n_2+1,1} - \eta_1(n_1 + 1)^2\delta_{n_1+1,1} - \eta_2(n_2 + 1)^2\delta_{n_2+1,1} \right] Y_3(t) \\
&\quad - i(-1)^{n_1}\Omega\delta_{n_1-1,0}\delta_{n_2+1,1}\sqrt{n_1(n_2 + 1)}Y_1(t) + i(-1)^{n_1}\Omega\delta_{n_1+1,1}\delta_{n_2-1,0}\sqrt{(n_1 + 1)n_2}Y_2^*(t).
\end{aligned}$$

To proceed we solve the equations for Y_1, Y_2, Y_3 in the steady state, assuming that the diagonal matrix elements are time constant in time over the lifetime of the off-diagonal matrix elements. This is the adiabatic approximation. These steady state values are then substituted back into the equation for the diagonal matrix elements to obtain a classical jump process master equation to describe sequential tunnelling. The algebra is tedious, so we will not give details. The result is

$$\begin{aligned}
& \frac{d}{dt}P(n_1, n_2, t) \\
&= -\gamma_L[(n_1 + 1)\delta_{n_1,0} - \gamma_R n_2 \delta_{n_2,1}]P(n_1, n_2, t) \\
&+ \delta_{n_1,1}\gamma_L n_1 P(n_1 - 1, n_2, t) + \delta_{n_2,0}\gamma_R(n_2 + 1)P(n_1, n_2 + 1, t) \\
&- 2\Omega^2\{\delta_{n_1,0}\delta_{n_2,1}(n_1 + 1)n_2 \frac{(a_{22}a_{33} - a_{23}a_{32})}{D}[P(n_1 + 1, n_2 - 1, 0) - P(n_1, n_2, 0)] \\
&+ \delta_{n_1,1}\delta_{n_2,0}n_1(n_2 + 1) \frac{(a_{11}a_{33} - a_{13}a_{31})}{D}[P(n_1 - 1, n_2 + 1, 0) - P(n_1, n_2, 0)]\}.
\end{aligned}$$

where D is given by

$$D = a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{13}a_{22}a_{31} \quad (34)$$

with

$$a_{11} = -\frac{\gamma_L}{2}(n_1 + 1)\delta_{n_1,0} - \frac{\gamma_R}{2}n_2\delta_{n_2,1} - \eta_1[n_1^2\delta_{n_1,1} + (n_1 + 1)^2\delta_{n_1,0}] - \eta_2n_2^2\delta_{n_2,1}$$

$$a_{13} = (-1)^{n_1}\Omega\delta_{n_1,1}\delta_{n_2,0}\sqrt{n_1(n_2 + 1)} = -a_{31}$$

$$a_{22} = -\frac{\gamma_L}{2}[(n_1 + 1)\delta_{n_1,0} + n_1\delta_{n_1,1}] - \frac{\gamma_R}{2}[n_2\delta_{n_2,1} + (n_2 + 1)\delta_{n_2,0}]$$

$$-\eta_1n_1^2\delta_{n_1,1} - \eta_2[n_2^2\delta_{n_2,1} + (n_2 + 1)^2\delta_{n_2,0}]$$

$$a_{23} = -(-1)^{n_1}\Omega\delta_{n_1,0}\delta_{n_2,1}\sqrt{(n_1 + 1)n_2} = -a_{32}$$

$$a_{33} = -\frac{\gamma_L}{2}n_1\delta_{n_1,1} - \frac{\gamma_R}{2}(n_2 + 1)\delta_{n_2,0} - \eta_1(n_1 + 1)^2\delta_{n_1,0} - \eta_2(n_2 + 1)^2\delta_{n_2,0}$$

In addition to the incoherent tunnelling of electrons between the wells and the external reservoirs, we now have incoherent (sequential) tunnelling between the two wells at rates determined by $\frac{\Omega^2}{\eta_i}$. The form of this equation corresponds to the sequential tunnelling master equation obtained by Carlos Egues et al [16]. We have thus shown that, in the limit of strong decoherence induced by elastic scattering of the bound states, a population master equation may describe sequential tunnelling in the device. This will be the appropriate limit in the case that $\eta_i \gg \Omega$. However future quantum nanostructures devices are likely to operate

in the opposite limit. In that case our method is ideally suited for determining the device characteristics.

IV. SUMMARY

We have shown how the quantum theory of open systems, formulated as a quantum stochastic process, enables the current noise spectrum to be calculated for mesoscopic tunnelling devices. Our approach explicitly treats quantum noise properties of the charge carriers, and gives a simple intuitive picture to understand the results. As fabrication technology develops, quantum noise limited networks of *coherent* tunnelling devices, such as quantum dots and quantum point contacts, will become increasingly important. Such coherently coupled devices are essential for the implementation of a quantum computer, which must operate reversibly [21]. The full operator master equation methods we have demonstrated here provide a powerful description, including both diagonal and off-diagonal matrix elements in the same equation.

Our model does not treat the transverse unbound modes in the well of a realistic resonant tunnelling device. These can easily be incorporated by additional states in the well and additional jump process channels in the master equation. We have not done that here as we sought to derive the irreducible level of current noise in tunnelling devices. Our model may in fact apply to very tightly confined quantum dot structures which could conceivably be fabricated with a single bound well states at donor impurities. Further extensions of the model are also needed to treat the case where the well state is just below the Fermi level in the collector in which case the current noise acquire an additional temperature dependent classical component. These more general cases will be treated in a larger publication.

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In this appendix we derive the master equation describing elastic scattering of the quasi-bound states of the well which cause a dephasing of the electron quasi-bound states but do not change their populations. The Hamiltonian for double-well system in Schroedinger picture is

$$H = H_0 + H_T + H_{scat} \quad (\text{A1})$$

$$H_0 = \sum_{n=1}^2 \varepsilon_n c_n^\dagger c_n + \sum_k \varepsilon_k^E a_k^\dagger a_k + \sum_p \varepsilon_p^C b_p^\dagger b_p + \sum_q \omega_q a_q^\dagger a_q + \Omega(c_1^\dagger c_2 + c_2^\dagger c_1) \quad (\text{A2})$$

$$H_T = \sum_k (T_{Ek} c^\dagger a_k + T_{Ek}^* a_k^\dagger c) + \sum_p (T_{Cp} b_p^\dagger c + T_{Cp}^* c^\dagger b_p) \quad (\text{A3})$$

$$H_{scat} = \sum_{n=1}^2 c_n^\dagger c_n \Gamma_n \quad (\text{A4})$$

where

$$\Gamma_1 = \sum_q M_q (\alpha_q^\dagger + \alpha_q) \quad (\text{A5})$$

$$\Gamma_2 = \sum_q M_q (\beta_q^\dagger + \beta_q) \quad (\text{A6})$$

where α_q, β_q are Bose destruction operators describing independent reservoir oscillators. Note that each bound state in the well is coupled to an independent reservoir. This assumes that there are no correlations between well states due to the dephasing that takes place through elastic collisions.

We will only consider here the derivation of the master equation arising from the elastic scattering of bound states and the harmonic oscillator reservoirs. The relevant part of the master equation is [13]

$$\frac{d\rho(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t d\tau Tr_B [H_{scat}(t), [H_{scat}(\tau), \rho(\tau) \otimes \rho_B]] \quad (\text{A7})$$

where ρ_B is the equilibrium state of the bath, and where Tr_B means to trace over the bath variables. This equation is based on a second order expansion in the interaction energy

between the reservoir states and the bound states of the well. We have also assumed that the system and bath states are decorrelated very rapidly on the time scale of interest in the system, so that the bath remains close to its equilibrium state. The bath Hamiltonian is

$$H_B = \sum_q \omega_q a_q^\dagger a_q \quad (\text{A8})$$

It will only be necessary to consider one of the bath-well state coupling terms in the scattering Hamiltonian. The relevant part of the master equation in the interaction picture is

$$\begin{aligned} \frac{d\rho(t)}{dt} = & -\frac{1}{\hbar^2} \int_0^t d\tau \text{Tr}_B \{ [c_n^\dagger c_n \sum_{q'} M_{q'} (\alpha_{q'}^\dagger e^{i\omega_{q'} t} + \alpha_{q'} e^{-i\omega_{q'} t}), \\ & [c_n^\dagger c_n \sum_q M_q (\alpha_q^\dagger e^{i\omega_q \tau} + \alpha_q e^{-i\omega_q \tau}), \rho(\tau) \otimes \rho_B]] \} \end{aligned} \quad (\text{A9})$$

We now define,

$$E \equiv c_n^\dagger c_n \sum_{q'} M_{q'} (\alpha_{q'}^\dagger e^{i\omega_{q'} t} + \alpha_{q'} e^{-i\omega_{q'} t}) \quad (\text{A10})$$

$$F \equiv c_n^\dagger c_n \sum_q M_q (\alpha_q^\dagger e^{i\omega_q(t-\tau)} + \alpha_q e^{-i\omega_q(t-\tau)}) \quad (\text{A11})$$

Therefore

$$\begin{aligned} \frac{d\rho(t)}{dt} = & -\frac{1}{\hbar^2} \int_0^t d\tau \text{Tr}_B \{ EF\rho(\tau) \otimes \rho_B - E\rho(\tau) \otimes \rho_B F \\ & - F\rho(\tau) \otimes \rho_B E + \rho(\tau) \otimes \rho_B FE \} \end{aligned} \quad (\text{A12})$$

The state of the reservoirs is taken to be a thermal state at temperature T , thus

$$\text{Tr}_B [\alpha_q \alpha_{q'} \rho_B] = \text{Tr}_B [\alpha_q^\dagger \alpha_{q'}^\dagger \rho_B] = 0 \quad (\text{A13})$$

$$\text{Tr}_B [\alpha_q^\dagger \alpha_{q'} \rho_B] = \delta_{qq'} \frac{1}{e^{E_q/k_B T} - 1} \quad (\text{A14})$$

The first term on the right hand of the equation (A12)

$$\begin{aligned} & \int_0^t d\tau \text{Tr}_B EF\rho(t) \otimes \rho_B \\ = & \int_0^t d\tau \sum_{qq'} M_q M_{q'} \delta_{qq'} \left[\frac{1}{e^{E_q/k_B T} - 1} e^{i[(\omega_{q'} - \omega_q)t + \omega_q \tau]} \right] \end{aligned}$$

$$\begin{aligned}
& + (1 + \frac{1}{e^{E_q/k_B T} - 1} e^{i[(\omega_q - \omega_{q'})t - \omega_q \tau]}) (c_n^\dagger c_n)^2 \rho \\
& = \int_0^t d\tau \sum_q |M_q|^2 [\frac{1}{e^{E_q/k_B T} - 1} e^{i\omega_q \tau} + (1 + \frac{1}{e^{E_q/k_B T} - 1}) e^{-i\omega_q \tau}] (c_n^\dagger c_n)^2 \rho \\
& = \sum_q |M_q|^2 [\frac{\sin(\omega_q t)}{\omega_q} (1 + \frac{2}{e^{E_q/k_B T} - 1}) + i \frac{\cos(\omega_q t) - 1}{\omega_q}] (c_n^\dagger c_n)^2 \rho \\
& = (\eta_n + i\xi_n) (c_n^\dagger c_n)^2 \rho
\end{aligned} \tag{A15}$$

Where

$$\eta_n \equiv \sum_{q'} |M_q|^2 \frac{\sin(\omega_q t)}{\omega_q} (1 + \frac{2}{e^{E_q/k_B T} - 1}) \tag{A16}$$

$$\xi_n \equiv \sum_{q'} |M_q|^2 \frac{\cos(\omega_q t) - 1}{\omega_q} \tag{A17}$$

Similarly,

$$\begin{aligned}
& - \int_0^t d\tau \text{Tr}_B E \rho(\tau) \otimes \rho_B F \\
& = -(\eta_n - i\xi_n) c_n^\dagger c_n \rho c_n^\dagger c_n
\end{aligned} \tag{A18}$$

$$\begin{aligned}
& - \int_0^t d\tau \text{Tr}_B F \rho(\tau) \otimes \rho_B E \\
& = -(\eta_n + i\xi_n) c_n^\dagger c_n \rho c_n^\dagger c_n
\end{aligned} \tag{A19}$$

$$\begin{aligned}
& \int_0^t d\tau \text{Tr}_B \rho(\tau) \otimes \rho_B F E \\
& = (\eta_n - i\xi_n) \rho (c_n^\dagger c_n)^2
\end{aligned} \tag{A20}$$

The coefficients η_n, ξ_n appear to be time dependant, but under reasonable physical assumptions are time independant [13]. These assumptions are, firstly that t is assumed to be a time scale over which the system operators vary significantly. On this time scale bath correlation functions decay rapidly. Secondly, that the bath is at finite temperature and there is significant excitation above the reservoir ground state. Finally that the coupling constants M_q are independent of q up to some large cut-off wave number. Under these

assumptions these coefficients can be evaluated in the limit of $t \rightarrow \infty$. We refer the reader to reference [13] for more details.

The total contribution from the scattering term to the master equation is therefore by substituting equations (A15) and (A18 -A20) and corresponding terms for the second well into equation (A12):

$$\frac{d\rho(t)}{dt} = \sum_{n=1}^2 \eta_n [c_n^\dagger c_n, [c_n^\dagger c_n, \rho]] + \frac{i\xi}{\hbar^2} \sum_{n=1}^2 [c_n^\dagger c_n, \rho] \quad (\text{A21})$$

The effect of the term $i\xi$ is to add a small perturbation to the energy of each quasi-bound well state and is equivalent to the Lamb shift term in atomic physics.

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FIGURES

FIG. 1. The current Fano factor $\frac{S(\omega)}{2e^2\hbar\omega}$ versus normalised frequency ω/γ_e in case 1. All parameters are normalised by γ_e . The corresponding parameters $(\eta_e/\gamma_e, \omega/\gamma_e)$ for the curves are from the top: Dotted:(0.5, 0.1); Dot-dash:(0.5, 0.2); Solid:(0.5, 0.24).

FIG. 2. The current Fano factor versus normalised frequency (ω/γ_e) in case 2. All parameters are normalised by γ_e . The corresponding parameters $(\eta_e/\gamma_e, \Omega/\gamma_e)$ for the curves are from the top: Dotted:(0, 0.2); Dot-dash:(0.4, 0.4); Solid:(0.5, 0.5).

FIG. 3. The comparison of influences of the elastic scattering and the coherent tunnelling. The corresponding parameters $(\eta_e/\gamma_e, \Omega/\gamma_e)$ for the curves are from the top: (a):(0.6, 0.1); (b):(0.0, 0.2); (c):(0.2, 0.5); (d):(0, 0.645).

FIG. 4. The current Fano-factors versus normalized frequency for double well structures. The normalized parameter Ω/γ_e for the curves are from top: 0.2 dash line, 0.645 dot-dash line, 5.0 solid line.

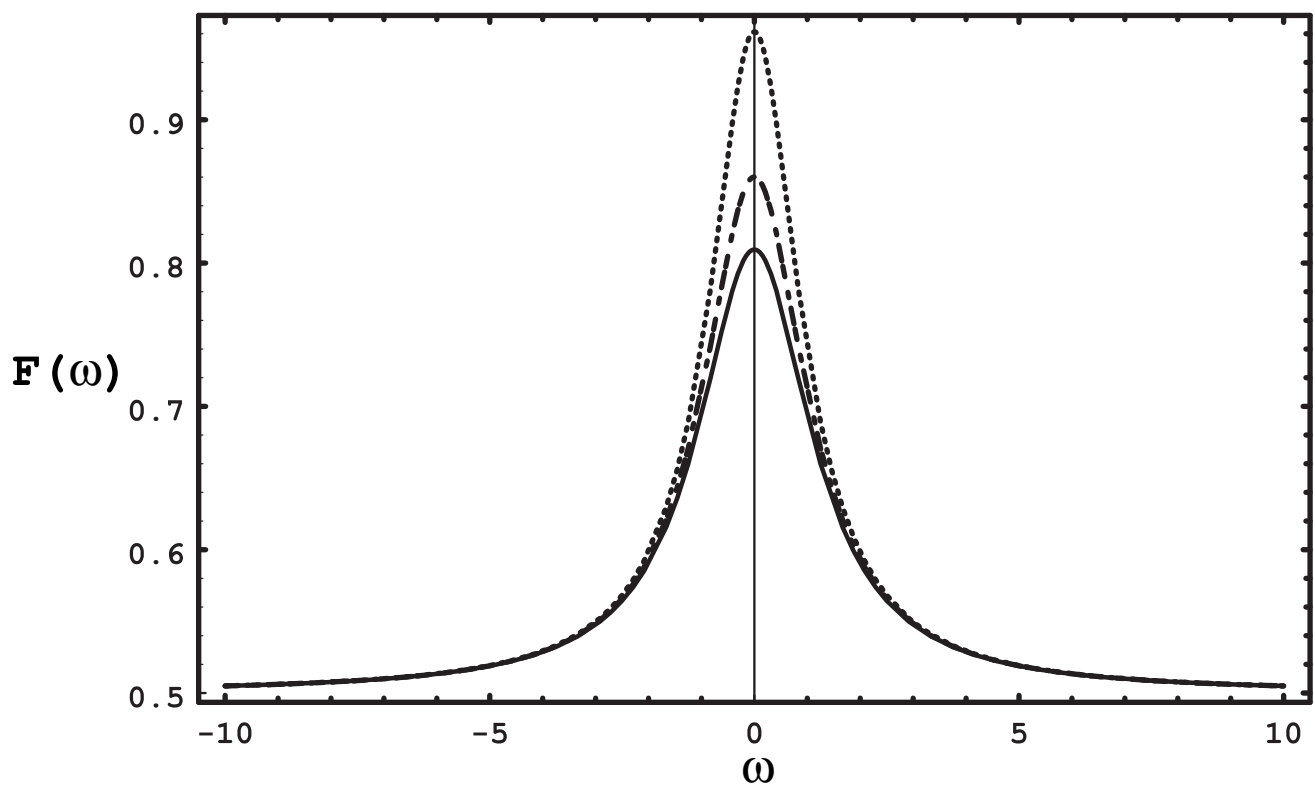


figure 1

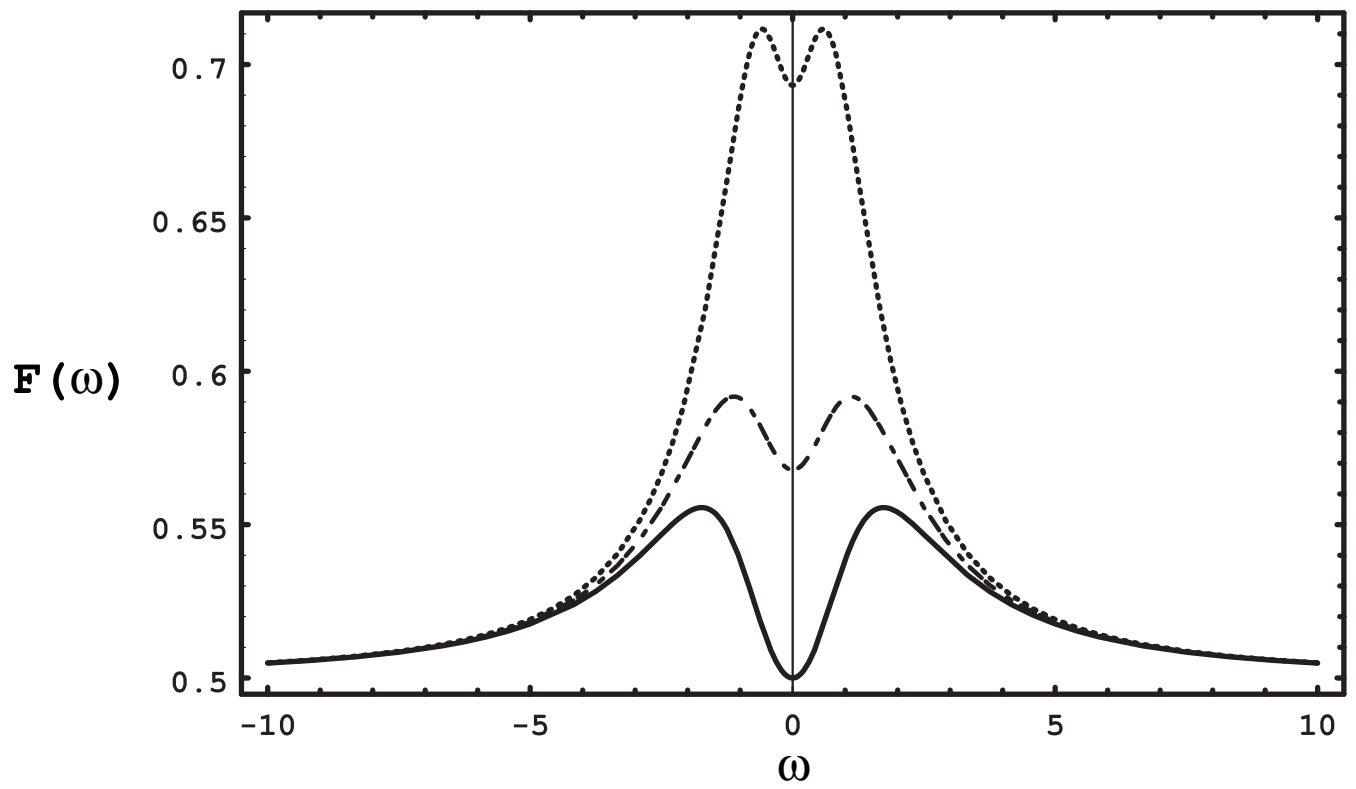


figure 2

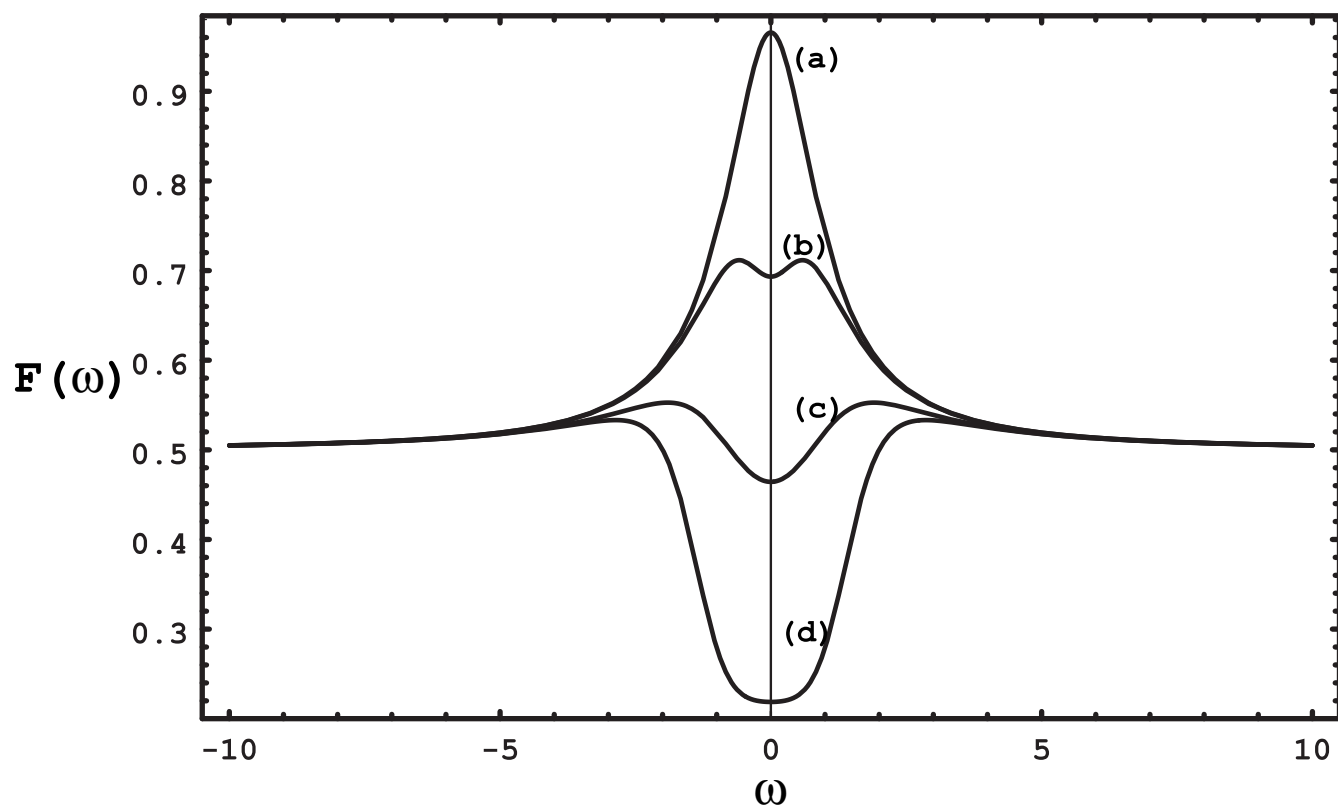


figure 3

